
About PCGEMS User's Guide

Abstract

The Personal Computer Version of the Graphical Exposure Modeling System (GEMS), called PCGEMS, is a complete information management tool designed to help you in performing exposure assessment studies. With PCGEMS, you may easily estimate chemical properties and perform simulation studies of chemical release in air, soil and groundwater systems. To enhance and further evaluate these simulation studies of chemical release, you may draw upon datasets of information such as population distribution, weather and wind statistics, and varieties of soils native to the area that you are studying.

PCGEMS contains extensive user support and can assist you through every step of PCGEMS with help messages, instructions, and error messages. PCGEMS is also designed to interact extensively with GEMS which resides on the VAX Cluster of computers at Research Triangle Park, North Carolina. This allows you to call upon the resources of the EPA VAX Cluster to better support your studies.

This document guides you through the many functions that make up PCGEMS. It instructs you on how to load the system, how to best use the access the user instruction built into the system, and other general information about the system. With regard to the environmental modeling programs and chemical property estimation programs that make up the heart of the system, this guide explains the scope and capabilities of each

program as well as the type of input necessary to run them. This manual also illustrates and explains screens that appear if you choose any of the programs in the graphics option, the data management option, the utilities option, the risk exposure assessment option, and the communications option. Since PCGEMS can be used in conjunction with GEMS, information on whom to contact for help and information is also provided. The manual also describes the databases available in PCGEMS including the size, the variables in the database, the programs that access the database.

Table of Contents

About PCGEMS User's Guide	i
1. General Information	1-1
1.1 GEMS and PCGEMS: Interactive Relationship	1-3
1.2 Minimum System Requirements	1-5
1.3 Loading PCGEMS	1-6
1.4 Starting PCGEMS from the Hard Disk	1-27
1.5 Menu Design	1-27
1.6 Command Keys and Help Messages	1-32
1.7 Correcting and Reporting Bugs	1-35
2. Chemical Property Estimation	2-1
2.1 Selecting a Chemical Property Estimation Program	2-3
2.2 SMILES from CAS (SMIGET)	2-4
2.3 Retrieve Properties from the Title III Database (TITLE III)	2-11
2.4 Octanol/Water Coefficient (PCLOGP)	2-13
2.5 Chemical Property Estimation (PCCHEM)	2-24
2.6 Hydrolysis of Water (PCHYDRO)	2-40
2.7 Fate of Atmospheric Pollutants (PCFAP)	2-45
2.8 Draw SMILES Notation (DRAWSMI)	2-51
2.9 Run User-Installed Estimation Programs	2-56
3. Environmental Modeling	3-1
3.1 Selecting an Environmental Modeling Program	3-1

3.2 Industrial Source Complex Long-Term (ISCLT2) Model	3-3
1. Build ISCLT2 Input File (BUILDISC)	3-6
2. Run ISCLT2 (RUNISC)	3-12
3. Exposure and Risk Estimation (EXPRISK)	3-13
4. ISCLT2 Graphics (ISCGRAPH)	3-16
5. Terrain Utility (TERRAIN)	3-17
3.3 Single Source Gaussian Dispersion Algorithm (PTPLU)	3-19
3.4 Seasonal Soil Compartment Model (SESOIL)	3-24
1. Build SESOIL Model Input File (SEBUILD)	3-25
2. Run SESOIL Model (SERUN)	3-28
3. SESOIL Graphics (SEGRAPH)	3-29
4. Create AT123D Input Dataset from SESOIL Output (SEATLINK) .	3-29
3.5 Analytical Transient 1-2-3 Dimensional Model (AT123D)	3-30
1. Build AT123D Model Input File (BUILD123)	3-31
2. Run AT123D on the PC (PCAT123D)	3-32
3. AT123D Isopleth (ATISO)	3-33
3.6 Exposure Analysis Modeling System (EXAMS-II)	3-34
1. Build Chemical Data File (EXCHEM)	3-35
2. Build Environment Data File (ENVTEMP)	3-37
3. Build Loading Command File (EXLOAD)	3-38
4. Run EXAMS-II (RUNEX)	3-39
5. EXAMS - II Graphics (EXGRAPH)	3-40
3.7 ReachScan Model (REACHSCA)	3-41
3.8 Environmental Partitioning Model (ENPART)	3-44
1. Build ENPART Model Input File (BUILDENP)	3-46
2. Run ENPART on the PC (PCENPART)	3-49
3.9 Run User-Installed Modeling Programs	3-50
4. Data Management	4-1
4.1 Selecting a Data Management Program.	4-1
4.2 Census Data Retrieval Program (CENSUS)	4-2
1. Retrieve Census Data by Key Values	4-4
2. Retrieve Population Data by Location	4-12
3. Retrieve Population Data for TRI Facilities	4-14
4.3 List File Directory (XDIR)	4-15
4.4 Install the File Editor (XEDITOR)	4-17

4.6 File Format Conversion (XFORMAT)	4-19
1. Convert ASCII files to LOTUS Worksheets (ASC2LOT)	4-21
2. Convert ASCII Files to DIF Format Files (ASC2DIF)	4-24
3. Convert ASCII files to dBASE III files (ASC2DB)	4-25
4.7 Catalog Manager (CATMGR)	4-26
4.8 Run User-Installed Data Management Programs	4-33
 5. Graphics	5-1
5.1 Selecting a Graphics Program	5-1
5.2 Run the STARROSE Program (ROSE)	5-2
5.3 General Geographic Mapping Program	5-9
5.4 Run User-Installed Graphics Programs	5-38
 6. Communications	6-1
6.1 Selecting a Communications Program.	6-2
6.2 Run MS-KERMIT (MSKERMIT)	6-2
6.3 Run User-Installed Communications Program	6-6
 7. Utilities	7-1
7.1 Selecting a Utilities Program	7-2
7.2 Changing PCGEMS Configuration File (CRFIG)	7-2
7.3 Install a Non-PCGEMS Program (XINSTALL)	7-5
7.4 Run a Non-PCGEMS Program (XRUN)	7-7
7.5 DX DY Calculator (DXDYCALC)	7-8
7.6 Run User-Installed Utilities Programs	7-11
 8. PCGEMS Datasets	8-1
8.1 Census Population Block Group and Block Datasets	8-2
8.2 Geographic Mapping Boundary Datasets	8-3
8.3 Reach Trace Dataset	8-4
8.4 ReachScan Dataset	8-4
8.5 CAS Numbers/SMILES Dataset	8-5
8.6 STAR Dataset	8-6
8.7 Zipcode Dataset	8-6
8.8 GEMS CHEMEST Dataset	8-7
8.9 TITLE III Dataset	8-7

Appendix A. Glossary	A-1
Appendix B. References	B-1
Index	I-1

List of Figures

Figure 1-1. System Herald	1-21
Figure 1-2. Selection of Graphics Mode Menu	1-22
Figure 1-3. Path Specification Menu	1-23
Figure 1-4. Color Specification Menu - Page 1	1-25
Figure 1-5. Color Specifications Menu - Page 2	1-25
Figure 1-6. Example of PCGEMS Menu Design	1-28
Figure 1-7. Example of Array Editing Menu	1-31
Figure 1-8. Example of a Table Selection Menu	1-32
Figure 2-1. Chemical Property Estimation Selection Menu	2-3
Figure 2-2. SMIGET Output Options Menu	2-4
Figure 2-3. CAS Number Input Method Menu	2-5
Figure 2-4. Direct Entry of CAS Number Menu	2-7
Figure 2-5. File Name Entry Menu	2-8
Figure 2-6. Entry of CAS Number from File Menu	2-9
Figure 2-8. PCLOGP Output Options Menu	2-13
Figure 2-9. PCLOGP Output File Label Menu	2-14
Figure 2-10. PCCHEM Input Method Options Menu	2-15
Figure 2-11. Direct SMILES Notation Entry Menu	2-16
Figure 2-12. Direct CAS Number Entry Menu	2-18
Figure 2-13. SMILES Notations File Entry Menu	2-20
Figure 2-14. ELOGP Input File Menu	2-22
Figure 2-15 CAS Numbers File Name Menu	2-23
Figure 2-16. PCCHEM Output Options Menu	2-29
Figure 2-17. Output Control Options Menu	2-30

Figure 2-18. PCCHEM Input Methods Menu	2-31
Figure 2-19. Direct Input - Smiles Notation Menu	2-32
Figure 2-20. Property Estimator Indicator Menu	2-33
Figure 2-21. Log K _{ow} Value Menu	2-35
Figure 2-22. SMILES Notation File Entry Menu	2-36
Figure 2-23. Range of SMILES Structures Entry Menu	2-39
Figure 2-24. PCHYDRO Main Menu	2-42
Figure 2-25. PCFAP Main Menu	2-46
Figure 2-26. Build FAP Input File Menu	2-46
Figure 2-27. SMILES Notation - Direct Entry Menu	2-47
Figure 2-28. Calculate FAP from SMILES File Menu	2-48
Figure 2-29. PCFAP Output Options Menu	2-50
Figure 3-1. Environmental Modeling Selection Menu	3-1
Figure 3-2. Industrial Source Complex Long-Term (ISCLT2) Model	3-5
Figure 3-3. PTPLU Control Menu	3-23
Figure 3-4. SESOIL Model Menu	3-24
Figure 3-5. AT123D Model Menu	3-31
Figure 3-6. EXAMS-II Model Menu	3-35
Figure 3-7. ReachScan Opening Menu	3-43
Figure 3-8. Environmental Partitioning Model Menu	3-45
Figure 4-1. Data Management Selection Menu	4-2
Figure 4-2. Census Data Retrieval Menu	4-3
Figure 4-3. Selection of Key Variables Menu	4-4
Figure 4-4. Logical Option Selection Menu	4-7
Figure 4-5. Specification of Key Variable Values	4-8
Figure 4-6. Selection of Output Variables Menu	4-9
Figure 4-7. The Output Selection Menu	4-10
Figure 4-8. Block Group and Block datasets Path Entry Menu	4-12
Figure 4-9. Location Entry Menu	4-13
Figure 4-10. The Ring Distance Specification Menu	4-13
Figure 4-11. TRI Facility Entry Menu	4-15
Figure 4-12. Directory Nenu	4-16
Figure 4-13. Install Data Editor Menu	4-18
Figure 4-14. File Editing Menu	4-19
Figure 4-15. File Format Conversion Navigational Menu	4-20
Figure 4-16. ASCII to LOTUS Conversion Menu	4-21

Figure 4-17. ASCII to Lotus Ver 1.1 or 1.1A Menu	4-22
Figure 4-18. Data Description Field Menu (ASC2LOT)	4-22
Figure 4-19. ASCII to LOTUS Release 2 Menu	4-23
Figure 4-20. Convert an ASCII File to DIF File Menu	4-24
Figure 4-21. ASCII to dBASE III Conversion Menu	4-25
Figure 4-22. Data Field Description Menu (dBASE III)	4-26
Figure 4-23. Catalog Manager Menu	4-29
Figure 5-1. Main Graphics Menu	5-2
Figure 5-2. Rose Data Input Options Menu	5-3
Figure 5-3. Source Location Data Type Menu	5-4
Figure 5-4. Selection of ROSE Type Menu	5-5
Figure 5-6. Draw Rose From Manual Input Menu	5-7
Figure 5-7. Manual Input - Page 1	5-8
Figure 5-8. Manual Input - Page 2	5-8
Figure 5-9. Geographic Coverage Selection Menu	5-11
Figure 5-10. Continental U.S. Map Menu	5-13
Figure 5-11. EPA Region Selection Menu	5-14
Figure 5-12. State Selection Menu	5-15
Figure 5-13. County Selection Menu	5-16
Figure 5-14. Area by Center Location and Radius	5-17
Figure 5-15. Area by Latitude and Longitude Ranges Menu	5-18
Figure 5-16. Selection of Data Overlay Menu	5-19
Figure 5-17. Map Border Specification Menu	5-22
Figure 5-18. Define the Lat/Lon Grids Menu	5-23
Figure 5-19. Overlay River Reaches Menu	5-24
Figure 5-20. ReachScan Overlay Menu	5-25
Figure 5-21. Overlay Weather Stations Menu	5-27
Figure 5-22. Overlay Census Centroids Menu	5-28
Figure 5-23. Choropleth From An ASCII File Menu	5-29
Figure 5-24. Choropleth Stored Data Menu	5-30
Figure 5-25. Choropleth Classification Menu	5-31
Figure 5-26. Manual Input Choropleth	5-32
Figure 5-27. Choropleth Classifications Number Menu	5-33
Figure 5-28. Classification of Choropleth Data Menu	5-34
Figure 5-29. Point Overlay Menu	5-35
Figure 5-30 Map Annotation	5-35

Figure 5-31. Output Specification	5-36
Figure 6-1. Selecting a Communications Program	6-2
Figure 7-1. The Utilities Selection Menu	7-2
Figure 7-2. Selection of Graphic Modes Menu	7-3
Figure 7-3. Path Specification Menu	7-4
Figure 7-4. Color Specifications Menu - Page 1	7-4
Figure 7-5. Color Specification Menu - Page 2	7-5
Figure 7-6. Install a Non-PCGEMS Program Menu	7-6
Figure 7-7. Run a Non-PCGEMS Program Menu	7-7
Figure 7-8. Primary Source Location Method Menu	7-10

List of Tables

Table 2-1. Properties that may be used as input for environmental models	2-2
Table 2-2. Conversion of Units	2-34